OCR A Formulae

Module 2: Foundations in Chemistry

Atomic Structure and isotopes

number of neutrons = mass number – atomic number

Relative atomic mass = (mass of isotope 1 x abundance of isotope 1) + (mass of isotope 2 x abundance of isotope 2)/100

Amount of Substance

% atom economy = M_r of desired product/sum of M_r of all products x 100

% yield = actual mass/theoretical mass x 100

moles = mass/M_r

moles = concentration x volume/1000 (dm^3)

moles = volume/24 (dm^3) (gases) (vale in data sheet)

moles = number of particles/6.02 x 10^{23} (value in data sheet)

mol dm^{-3} x M_r → g dm^{-3}

PV = nRT (gases) where v is in m^3, T is in K and P is in Pa, R (in data sheet)

percentage error = uncertainty in instrument/value x 100

Physical Chemistry

Enthalpy Changes

ΔH = sum of bonds broken – sum of bonds made (mean bond enthalpies)

Q = mc ΔT where m = mass of water, c = 4.18 (in data sheet) and T is in K

Reaction Rates

Rate = 1/time

Rate = gradient of concentration-time curve

Equilibrium

$$aA + bB \rightleftharpoons cC + dD$$

$$K_c = \frac{[C]^c[D]^d}{[A]^a[B]^b}$$

Module 5: Physical Chemistry & Transition Elements

Rates

For A + B → C + D **rate = k[A][B]**

$k = \ln 2/t_{½}$ where $t_{½}$ = a half-life for a 1st order reaction

Arrhenius: **$k = Ae^{-Ea/RT}$**

$\ln k = \ln A - E_a/RT$ (both given in data sheet)

Equilibrium

Example:

$$CH_4(g) + H_2O(g) \rightleftharpoons CO(g) + 3H_2(g)$$

$$K_p = \frac{p(CO) \times p(H_2)^3}{p(CH_4) \times p(H_2O)}$$

Mole fraction = moles of one gas/moles of all the gases

Partial Pressure = mole fraction x total pressure

Total Pressure = sum of the partial pressures

Acids and Bases

$pH = -\log_{10} [H^+]$

$[H^+] = 10^{-pH}$

$K_w = [H^+][OH^-] = 1x10^{-14}\ mol^2dm^{-6}$ (at room temp) (value in data sheet)

$K_w = [H^+]^2$ (pure water)

% dissociation: H^+ concentration at equilibrium/the original acid concentration x 100

Expression and use in buffer calculations:

$$K_a = \frac{[H^+][A^-]}{[HA]}$$

Weak acid calculations:

$$K_a = \frac{[H^+]^2}{[HA]}$$

$pK_a = -log_{10}K_a$

$K_a = 10^{-pKa}$

Enthalpy, Entropy & Free Energy

ΔS = (sum of entropy of products) – (sum of entropy of reactants)

ΔH = (sum of enthalpy of products) – (sum of enthalpy of reactants)

$\Delta G = \Delta H - T\Delta S_{system}$

min. temp. = $\Delta H/\Delta S_{system}$

Electrode Potentials

$E_{cell} = E^\ominus$ of the more positive value – $E^\ominus$ of the more negative value

or

$E_{cell} = E^\ominus$ of the species being reduced – $E^\ominus$ of the species being oxidised